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Methyl 1*H*-1,2,3-triazole-4-carboxylate

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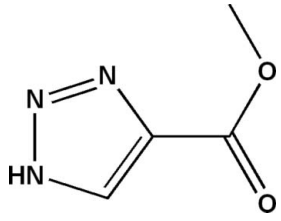
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.116; data-to-parameter ratio = 12.1.

The title compound, $C_4H_5N_3O_2$, features an essentially planar molecule (r.m.s. deviation for all non-H atoms = 0.013 Å). The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds and π–π stacking interactions (centroid–centroid distance 3.882 Å).

Related literature

For general background, see: Abu-Orabi *et al.* (1989); Fan & Katritzky (1996); Dehne (1994). For a related structure, see: Wang *et al.* (1998).



Experimental

Crystal data

$C_4H_5N_3O_2$
M_r = 127.11
Monoclinic, $P2_1/n$
a = 3.8823 (7) Å
b = 17.499 (3) Å
c = 8.8171 (17) Å
β = 100.938 (3)°
V = 588.12 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 290 (2) K
0.30 × 0.23 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.956, T_{max} = 0.977
4285 measured reflections
1098 independent reflections
917 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.06
1098 reflections
91 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3*N*···O1^{i}	0.896 (19)	1.980 (19)	2.8659 (19)	169.56 (18)

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1999) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2847).

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S1. Comment

Triazoles play an important role in pharmaceuticals, agrochemicals, dyes, photographic materials, and in corrosion inhibition (Fan & Katritzky, 1996; Dehne, 1994; Abu-Orabi *et al.*, 1989).

The crystal structure of the title compound is stabilized by intermolecular N—H···O hydrogen bonds and $\pi^{\cdots}\pi$ stacking interactions between the triazole rings at (symmetry operator 1+*X*,Y,*Z*; centroid-centroid distance 3.882 Å).

S2. Experimental

A mixture of methylpropiolate, 1 and trimethylsilylazide, 2 were heated at 100 °C till the completion of reaction, monitored by TLC. Then reaction mixture was cooled and methanol was added dropwise with cooling. The solid formed was allowed to stand for 30 min and filtered off, washed with ether, then with hexane. The product was then isolated as a colourless solid by column chromatography using 10% pet.ether/EtOAc. The single-crystal for X-ray structue anlaysis was obtained from ether solution by slow evaporation.

S3. Refinement

All the H atoms in (I) were positioned geometrically and refined using a riding model with C—H bond lengths of 0.93 Å and 0.97 Å for aromatic and for methyl H atoms respectively and U_{iso}(H) = 1.2U_{eq}(C) for all carbon bound H atoms.

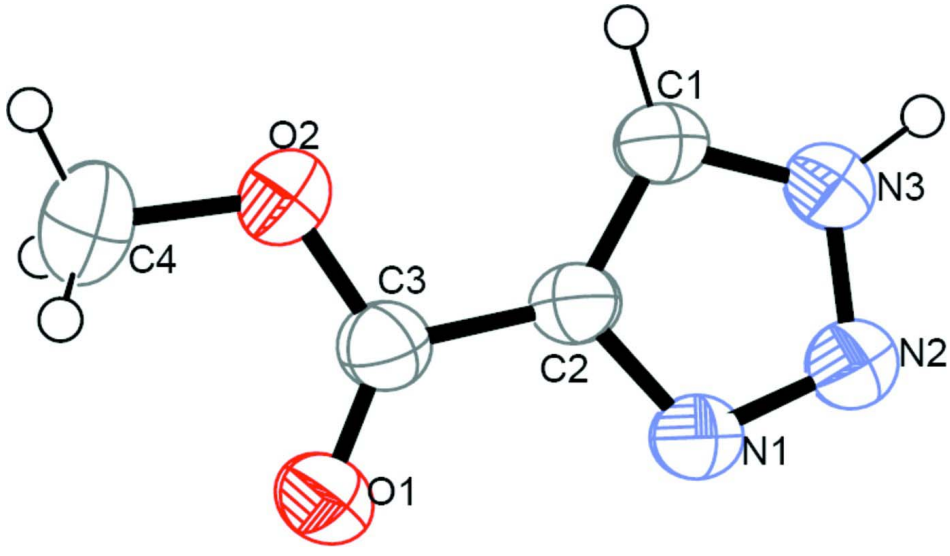

Figure 1

ORTEP diagram of the asymmetric unit of the title compound with 50% probability displacement ellipsoids.

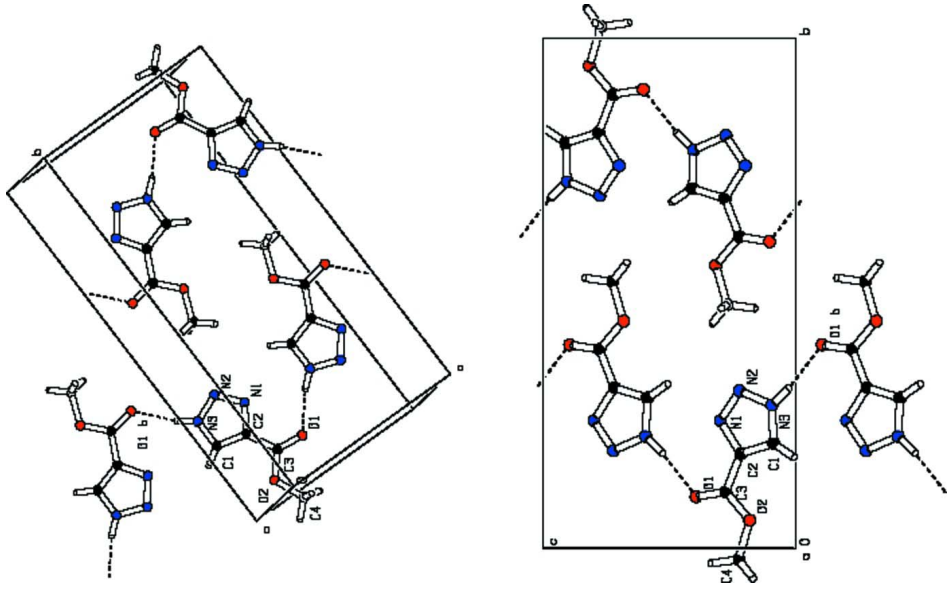

Figure 2

The crystal packing diagram of the title compound. The dotted lines indicate intermolecular N—H···O hydrogen bonds.

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Crystal data

$C_4H_5N_3O_2$
M_r = 127.11
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 3.8823 (7) Å
b = 17.499 (3) Å
c = 8.8171 (17) Å
β = 100.938 (3)°
V = 588.12 (19) Å^3
Z = 4
$F(000)$ = 264
D_x = 1.436 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1804 reflections
θ = 2.4–25.5°
μ = 0.12 mm^{-1}
T = 290 K
Block, pale yellow
0.30 × 0.23 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.956, T_{max} = 0.977
4285 measured reflections
1098 independent reflections
917 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 25.5°, θ_{min} = 2.3°
h = −4→4
k = −21→20
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.06
1098 reflections
91 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.085P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
H3N	0.668 (5)	0.1865 (11)	0.529 (2)	0.069 (6)*
H1	0.630 (5)	0.3213 (10)	0.510 (2)	0.067 (5)*
O1	0.2633 (4)	0.39888 (6)	0.89548 (14)	0.0672 (4)
O2	0.4220 (4)	0.44536 (7)	0.68279 (14)	0.0670 (4)
C3	0.3702 (4)	0.38941 (9)	0.77686 (18)	0.0502 (4)
N3	0.5970 (4)	0.21920 (8)	0.59504 (15)	0.0520 (4)
C2	0.4540 (4)	0.31459 (8)	0.71907 (16)	0.0440 (4)
N2	0.5029 (4)	0.19156 (8)	0.72315 (16)	0.0577 (4)
C1	0.5704 (4)	0.29447 (9)	0.58856 (18)	0.0495 (4)
N1	0.4149 (4)	0.25012 (7)	0.79947 (15)	0.0541 (4)
C4	0.3391 (8)	0.52244 (11)	0.7273 (3)	0.0937 (8)
H4A	0.0894	0.5296	0.7056	0.141*
H4B	0.4472	0.5590	0.6700	0.141*
H4C	0.4261	0.5295	0.8358	0.141*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0984 (10)	0.0524 (7)	0.0599 (8)	−0.0045 (6)	0.0379 (7)	−0.0077 (5)
O2	0.0959 (10)	0.0450 (7)	0.0671 (8)	0.0012 (6)	0.0330 (7)	0.0062 (5)
C3	0.0556 (9)	0.0481 (9)	0.0482 (9)	−0.0045 (7)	0.0137 (7)	−0.0012 (7)
N3	0.0643 (9)	0.0499 (8)	0.0443 (8)	0.0026 (6)	0.0167 (6)	−0.0038 (6)
C2	0.0478 (8)	0.0464 (8)	0.0384 (8)	−0.0034 (6)	0.0095 (6)	0.0015 (6)
N2	0.0754 (10)	0.0480 (8)	0.0532 (8)	0.0009 (6)	0.0213 (7)	0.0017 (6)
C1	0.0597 (10)	0.0499 (9)	0.0410 (9)	−0.0013 (7)	0.0152 (7)	0.0031 (7)
N1	0.0702 (9)	0.0480 (8)	0.0478 (8)	−0.0016 (6)	0.0207 (7)	0.0011 (5)
C4	0.134 (2)	0.0464 (11)	0.1117 (18)	0.0019 (11)	0.0499 (16)	0.0029 (11)

Geometric parameters (Å, º)

O1—C3	1.2075 (19)	C2—N1	1.3561 (19)
O2—C3	1.3231 (19)	C2—C1	1.360 (2)
O2—C4	1.458 (2)	N2—N1	1.3065 (19)
C3—C2	1.464 (2)	C1—H1	0.906 (19)
N3—C1	1.322 (2)	C4—H4A	0.9600

N3—N2	1.3416 (19)	C4—H4B	0.9600
N3—H3N	0.90 (2)	C4—H4C	0.9600
C3—O2—C4	116.63 (15)	N3—C1—C2	104.91 (14)
O1—C3—O2	124.02 (15)	N3—C1—H1	121.4 (12)
O1—C3—C2	124.05 (14)	C2—C1—H1	133.7 (12)
O2—C3—C2	111.92 (13)	N2—N1—C2	108.49 (13)
C1—N3—N2	111.36 (14)	O2—C4—H4A	109.5
C1—N3—H3N	129.6 (12)	O2—C4—H4B	109.5
N2—N3—H3N	119.0 (12)	H4A—C4—H4B	109.5
N1—C2—C1	108.37 (14)	O2—C4—H4C	109.5
N1—C2—C3	120.51 (13)	H4A—C4—H4C	109.5
C1—C2—C3	131.12 (14)	H4B—C4—H4C	109.5
N1—N2—N3	106.88 (13)		
C4—O2—C3—O1	−0.7 (3)	N2—N3—C1—C2	0.00 (17)
C4—O2—C3—C2	178.67 (17)	N1—C2—C1—N3	−0.01 (17)
O1—C3—C2—N1	−0.2 (2)	C3—C2—C1—N3	−179.24 (16)
O2—C3—C2—N1	−179.54 (14)	N3—N2—N1—C2	−0.03 (18)
O1—C3—C2—C1	178.95 (17)	C1—C2—N1—N2	0.03 (18)
O2—C3—C2—C1	−0.4 (2)	C3—C2—N1—N2	179.35 (13)
C1—N3—N2—N1	0.02 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*N*···O1^{i}	0.896 (19)	1.980 (19)	2.8659 (19)	169.56 (18)

Symmetry code: (i) *x*+1/2, −*y*+1/2, *z*−1/2.